# FINITE ELEMENTS IN FLUIDS

Homework 1 Unsteady Convection Diffusion Reaction Equation

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# 1. **Derivation**

Consider the transient convection-diffusion-reaction problem with the scalar unknown  $\rho$ , the convection velocity  $\boldsymbol{a}$ , the coefficient of diffusivity  $\nu > 0$ , the volumetric source term s and the reaction term  $\sigma$ .

$$\rho_t + \boldsymbol{a} \cdot \boldsymbol{\nabla} \rho - \boldsymbol{\nabla} \cdot (\nu \boldsymbol{\nabla} \rho) + \sigma \rho = s \text{ in } \Omega$$
(1.1)

with the boundary condition

$$\rho = 1 \quad \text{in } \Gamma_2$$
$$\rho = 0 \quad \text{in } \Gamma_4$$

The problem is solved using SUPG and GLS for the spatial discretization and Padé approximations using  $R_{1,1}$ ,  $R_{2,2}$  and  $R_{2,0}$  for the time derivative.

### 1.1 Weak Form

(1.1) gives the strong form of the problem. The equivalent weak form can be obtained by multiplying the equation with weighting function w and integration by parts. The trial solution space S consists function  $\rho$  defined on  $\Omega$  such that Dirichlet condition is satisfied. The space  $\mathcal{V}$  of the weighting function w is chosen such that w = 0 on  $\Gamma_D$ . The weak form will then be find  $u \in S$  such that

$$\int_{\Omega} w\rho_t \, \mathrm{d}\Omega + \int_{\Omega} w(\boldsymbol{a} \cdot \boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega - \int_{\Omega} w\boldsymbol{\nabla} \cdot (\nu\boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega + \int_{\Omega} w(\sigma\rho) \, \mathrm{d}\Omega = \int_{\Omega} ws \, \mathrm{d}\Omega \quad \forall w \in \mathcal{V}$$

Performing integration by parts and using the fact that w = 0 on  $\Gamma_D$ ,

$$\int_{\Omega} w\rho_t \, \mathrm{d}\Omega + \int_{\Omega} w(\boldsymbol{a} \cdot \boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{\nabla}w \cdot (\nu \boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega + \int_{\Omega} w(\sigma\rho) \, \mathrm{d}\Omega$$
$$= \int_{\Omega} ws \, \mathrm{d}\Omega + \int_{\Gamma_N} w(\nu \boldsymbol{\nabla}\rho \cdot \boldsymbol{n}) \, \mathrm{d}\Gamma \quad \forall w \in \mathcal{V}.$$
(1.2)

Introducing the compact form of (1.2) based on the integral forms defined in the following,

$$\int_{\Omega} w\rho_t \, \mathrm{d}\Omega = \left(w, \frac{\partial\rho}{\partial t}\right) \qquad \int_{\Omega} w(\boldsymbol{a} \cdot \boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega = \mathbf{c}(\boldsymbol{a}; w, \rho)$$

$$\int_{\Omega} \boldsymbol{\nabla}w \cdot (\nu \boldsymbol{\nabla}\rho) \, \mathrm{d}\Omega = \mathbf{a}(w, \rho) \qquad \int_{\Omega} w(\sigma\rho) \, \mathrm{d}\Omega = (w, \sigma\rho) \qquad (1.3)$$

$$\int_{\Omega} ws \, \mathrm{d}\Omega = (w, s) \qquad \int_{\Gamma_N} w(\nu \boldsymbol{\nabla}\rho \cdot \boldsymbol{n}) \, \mathrm{d}\Gamma = (w, h)_{\Gamma_N}$$

The compact form of the weak form can be written as,

$$\left(w,\frac{\partial\rho}{\partial t}\right) + \mathbf{c}(\boldsymbol{a};w,\rho) + \mathbf{a}(w,\rho) + (w,\sigma\rho) = (w,s) + (w,h)_{\Gamma_N}$$
(1.4)

Since there is no Neumann boundary condition in the problem stated in (1.1) the weak form becomes,

$$\left(w,\frac{\partial\rho}{\partial t}\right) + \mathbf{c}(\boldsymbol{a};w,\rho) + \mathbf{a}(w,\rho) + (w,\sigma\rho) = (w,s)$$
(1.5)

In addition, the weak form for the steady-state diffusion-convection-reaction problem can be written as,

$$\mathbf{c}(\boldsymbol{a}; \boldsymbol{w}, \boldsymbol{\rho}) + \mathbf{a}(\boldsymbol{w}, \boldsymbol{\rho}) + (\boldsymbol{w}, \sigma \boldsymbol{\rho}) = (\boldsymbol{w}, \boldsymbol{s}) \tag{1.6}$$

## 1.2 Padé approximation for temporal discretization

The strong form in (1.1) can be rewritten as

$$\rho_t + \mathcal{L}(\rho) = s \tag{1.7}$$

where the spatial differential operator is defined as,

$$\mathcal{L} := \boldsymbol{a} \cdot \boldsymbol{\nabla} - \boldsymbol{\nabla} \cdot (\nu \boldsymbol{\nabla}) + \sigma \tag{1.8}$$

## Two stage explicit scheme, $R_{2,0}$

For two stage explicit scheme,

$$R_{2,0}(z) = 1 + z + \frac{z^2}{2} \quad \text{where} \quad z = \Delta t \frac{\partial}{\partial t} \tag{1.9}$$

Using Taylor series expansion to obtain the discretization of the temporal derivatives we get

$$\rho(t^{n+1}) = \rho(t^n) + \Delta t \frac{\partial}{\partial t} \left( \rho + \frac{\Delta t}{2} \frac{\partial \rho}{\partial t} \right) + \mathcal{O}(\Delta t^3)$$
(1.10)

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which yields the two stage explicit method as

$$\rho^{n+1/2} = \rho^n + \frac{\Delta t}{2} \frac{\partial \rho^n}{\partial t}$$

$$\rho^n = \rho^n + \Delta t \frac{\partial \rho^{n+1/2}}{\partial t}$$
(1.11)

By replacing the time derivatives in (1.7) and (1.8), the Galerkin formulation of two-stage explicit Padé methods is,

$$\begin{pmatrix} w, \rho^{n+1/2} \end{pmatrix} = (w, \rho^n) + \frac{\Delta t}{2} \left[ (w, s^n) - \mathbf{c}(\mathbf{a}; w, \rho^n) - \mathbf{a}(w, \rho^n) - (w, \sigma \rho^n) \right] \begin{pmatrix} w, \rho^{n+1} \end{pmatrix} = (w, \rho^n) + \frac{\Delta t}{2} \left[ (w, s^{n+1/2}) - \mathbf{c}(\mathbf{a}; w, \rho^{n+1/2}) - \mathbf{a}(w, \rho^{n+1/2}) - (w, \sigma \rho^{n+1/2}) \right] (1.12)$$

#### One stage second order scheme, $R_{1,1}$

For one stage implicit scheme,

$$R_{1,1}(z) = \frac{1+z/2}{1-z/2} \quad \text{where} \quad z = \Delta t \frac{\partial}{\partial t}$$
(1.13)

Using Taylor series expansion to obtain the discretization of the temporal derivatives we get

$$\rho(t^{n+1}) = \frac{1+z/2}{1-z/2}\rho(t^n) \tag{1.14}$$

rearranging this we get

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} - \frac{1}{2} \frac{\partial \left(\rho^{n+1} - \rho^n\right)}{\partial t} = \frac{\partial \rho^n}{\partial t}$$
(1.15)

The compact form of the implicit Padé scheme can be written as,

$$\frac{\Delta\rho}{\Delta t} - \mathbf{W}\frac{\partial\Delta\rho}{\partial t} = \mathbf{w}\frac{\partial\rho^n}{\partial t}$$
(1.16)

The time derivatives in (1.16) can be replaced by spatial derivatives using the rewritten strong form in (1.7) and (1.8). For the problem stated in (1.16) becomes,

$$\frac{\Delta\rho}{\Delta t} - \mathbf{W}\mathcal{L}(\Delta\rho) = \mathbf{w}\left[s^n - \mathcal{L}(\rho^n)\right] + \mathbf{W}\Delta s \tag{1.17}$$

For one stage second order scheme,

$$\Delta \rho = \rho^{n+1} - \rho^n \qquad \mathbf{w} = 1$$
$$\mathbf{W} = \frac{1}{2} \qquad \Delta s = s^{n+1} - s^n \qquad (1.18)$$

#### Two stage fourth order scheme, $R_{2,2}$

For two stage implicit scheme,

$$R_{2,2}(z) = \frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} - \frac{z^2}{12}} \quad \text{where} \quad z = \Delta t \frac{\partial}{\partial t}$$
(1.19)

Rearranging terms in the above equation we obtain the same compact form as in (1.17) with

$$\Delta \rho = \begin{bmatrix} \rho^{n+1/2} - \rho^n \\ \rho^{n+1} - \rho^{n+1/2} \end{bmatrix} \begin{bmatrix} s^{n+1/2} - s^n \\ s^{n+1} - s^{n+1/2} \end{bmatrix}$$
$$\mathbf{W} = \frac{1}{24} \begin{bmatrix} 7 & -1 \\ 13 & 5 \end{bmatrix} \qquad \mathbf{W} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
(1.20)

## **1.3** Stabilization techniques

In order to stabilize the convective term and guarantee the solution for the differential equation is also a solution for the weak form given in (1.4) an extra term is added over the element interiors in (1.4). This term is a function of the residual of the differential equation to ensure consistency. The weak form with the stabilization term can be written as

$$\left(w,\frac{\partial\rho}{\partial t}\right) + \mathbf{c}(\boldsymbol{a};w,\rho) + \mathbf{a}(w,\rho) + (w,\sigma\rho) + \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w)\tau \mathcal{R}(\rho) \,\mathrm{d}\Omega = (w,s) \quad (1.21)$$

The weak form for the compact implicit Paé given in (1.16) can be obtained as,

$$\left(w, \frac{\Delta\rho}{\Delta t}\right) - \left(w, \mathbf{W}\frac{\partial\Delta\rho}{\partial t}\right) + \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w)\tau \mathcal{R}(\Delta\rho) \,\mathrm{d}\Omega = \left(w, \mathbf{w}\frac{\partial\rho^{n}}{\partial t}\right)$$
(1.22)

where  $\mathcal{P}(w)$  is a certain operator depends on different stabilizing methods,  $\tau$  is the stabilization parameter and  $\mathcal{R}(\rho)$  is the residual of the differential equation, which for the unsteady convective-diffusion reaction problem is,

$$\mathcal{R}(\rho) = \rho_t + \boldsymbol{a} \cdot \boldsymbol{\nabla} \rho - \boldsymbol{\nabla} \cdot (\nu \boldsymbol{\nabla} \rho) + \sigma \rho - s$$

For the compact implicit Padé,  $\mathcal{R}(\rho)$  is obtained as,

$$\mathcal{R}(\rho) = \frac{\Delta \rho}{\Delta t} - \mathbf{W} \frac{\partial \Delta \rho}{\partial t} - \mathbf{w} \frac{\partial \rho^n}{\partial t}$$

#### The SUPG method

For the SUPG method, the stabilization operator  $\mathcal{P}(w)$  is obtained as,

$$\mathcal{P}(w) := \boldsymbol{a} \cdot \boldsymbol{\nabla} w \tag{1.23}$$

Or for the multistage scheme,

$$\mathcal{P}(w) := \mathbf{W}(\boldsymbol{a} \cdot \boldsymbol{\nabla})w \tag{1.24}$$

#### The GLS method

For the GLS method, the stabilization operator  $\mathcal{P}(w)$  is obtained as,

$$\mathcal{P}(w) := \frac{\partial w}{\partial t} + \boldsymbol{a} \cdot \boldsymbol{\nabla} w - \boldsymbol{\nabla} \cdot (\boldsymbol{\nu} \boldsymbol{\nabla} w) + \sigma w$$
(1.25)

Or for the multistage scheme,

$$\mathcal{P}(w) := \frac{w}{\Delta t} + \mathbf{W} \left[ \mathbf{a} \cdot \nabla w - \nabla \cdot (\nu \nabla w) + \sigma w \right]$$
(1.26)

# 1.4 Discretization

Discretization on the unknown  $\rho$  and testing function w is given as follows,

$$\rho(x) = \sum_{j}^{n_{elem}} \rho_j N_j(x)$$
$$w(x) = \sum_{i}^{n_{elem}} w_i N_i(x)$$

Representation of matrices to simplify the writting of equations are given below.

$$\mathbf{M} = \int_{\Omega^{e}} N_{i} N_{j} d\Omega$$

$$\mathbf{C} = \int_{\Omega^{e}} N_{i} (a \cdot \nabla N_{j}) d\Omega$$

$$\mathbf{B} = \int_{\Omega^{e}} (a \cdot \nabla N_{i}) (a \cdot \nabla N_{j}) d\Omega$$

$$\mathbf{K} = \int_{\Omega^{e}} \nabla N_{i} \cdot (v \nabla N_{j}) d\Omega$$

$$\mathbf{D} = \int_{\Omega^{e}} (a \cdot \nabla N_{i}) N_{j} d\Omega$$

$$\mathbf{f} = \int_{\Omega^{e}} s N_{i} d\Omega$$
(1.27)

#### 1.4.1 Steady state problem

The matrix representation of the weak form (1.6) of the steady state problem can be written as

$$(\mathbf{C} + \mathbf{K} + \sigma \mathbf{M})\rho = \mathbf{f} \tag{1.28}$$

Considering the SUPG and GLS stabilization techniques with linear elements and neglecting the diffusion term, the stabilization terms can be written as following,

$$\begin{aligned} \text{SUPG} : \quad & \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho) d\Omega = (a \cdot \nabla w) \tau (a \cdot \nabla \rho - \nabla \cdot (v \nabla \rho) + \sigma \rho - s) \\ \text{GLS} : & \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho) d\Omega = ((a \cdot \nabla)w - \nabla \cdot (v \nabla w) + \sigma w) \tau (a \cdot \nabla \rho - \nabla \cdot (v \nabla \rho) + \sigma \rho - s) \end{aligned}$$

In the matrix form the above equations of SUPG and GLS can be written as,

SUPG 
$$(\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D}))\rho = \mathbf{f} + \tau s \mathbf{D}$$
  
GLS  $(\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D} + \sigma \mathbf{C} + \sigma^2 \mathbf{M}))\rho = \mathbf{f} + \tau s (\mathbf{D} + \sigma \mathbf{M})$ 

Finally the linear system to be solved can be written as the following,

$$\mathbf{A} \rho = \mathbf{F}$$

Galerkin method

$$\mathbf{A} = \mathbf{C} + \mathbf{K} + \sigma \mathbf{M}$$
 and  $\mathbf{F} = \mathbf{f}$ 

SUPG

$$\mathbf{A} = \mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D})$$
 and  $\mathbf{F} = \mathbf{f} - \tau s \mathbf{D}$ 

 $\mathbf{GLS}$ 

$$\mathbf{A} = \mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D} + \sigma \mathbf{C} + \sigma^2 \mathbf{M}) \text{ and } \mathbf{F} = \mathbf{f} - \tau s (\mathbf{D} + \sigma \mathbf{M})$$

#### 1.4.2 Explicit Pade

The two stage explicit Pade  $R_{2,0}$  is presented in (1.12). By using the matrix abbreviation defined in (1.27), the matrix form for the simple Galerkin approximation can be written as follows,

$$\frac{2}{\Delta t} \mathbf{M} \Delta \rho_1 = \mathbf{f}^n - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^n$$
$$\frac{1}{\Delta t} \mathbf{M} \Delta \rho_2 = \mathbf{f}^{n+1/2} - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^{n+1/2}$$
(1.29)

where  $\Delta \rho_1 = \rho^{n+1/2} - \rho^n$  and  $\Delta \rho_2 = \rho^{n+1} - \rho^n$ .

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Now, consider the two different types of stabilization techniques, that is SUPG and GLS. The diffusion term is neglected as the linear elements are used. The stabilization of the first step of  $R_{2,0}$  is written as follows,

$$\begin{aligned} \text{SUPG} : & \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho_{1}) d\Omega = (a \cdot \Delta w) \tau \Big( \frac{\Delta \rho_{1}}{\Delta t} + a \cdot \nabla \rho^{n} - \nabla \cdot (v \nabla \rho^{n}) + \sigma \rho^{n} - s \Big) \\ \text{GLS} : & \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho_{1}) d\Omega = \Big( \frac{w}{\Delta t} + a \cdot \nabla) w - \nabla \cdot (v \nabla w) + \sigma w \Big) \tau \\ & \Big( \frac{\Delta \rho_{2}}{\Delta t} + a \cdot \nabla \rho^{n} - \nabla \cdot (v \nabla \rho^{n}) + \sigma \rho^{n} - s^{n} \Big) \end{aligned}$$

Replacing  $\rho^n$  with  $\rho^{n+1/2}$  and by representing in the matrix form as described in the (1.27), the stability terms are written as follows,

SUPG : 
$$\frac{1}{\Delta t} (2\mathbf{M} + \tau \mathbf{D}) \Delta \rho_1 = \mathbf{f}^n - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D})) \rho^n + \tau s \mathbf{D}$$
$$\frac{1}{\Delta t} (2\mathbf{M} + \tau \mathbf{D}) \Delta \rho_2 = \mathbf{f}^{n+1/2} - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D})) \rho^{n+1/2} + \tau s \mathbf{D}$$

$$\begin{aligned} \text{GLS}: \quad \frac{1}{\Delta t} \Big( 2\mathbf{M} + \tau \Big( \frac{\mathbf{M}}{\Delta t} + \mathbf{D} + \sigma \mathbf{M} \Big) \Big) \Delta \rho_1 &= \mathbf{f}^n - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^n \\ &+ \tau \Big( \frac{1}{\Delta t} \mathbf{C} + \mathbf{B} + \sigma \mathbf{C} + \frac{\sigma}{\Delta t} \mathbf{M} + \sigma \mathbf{D} + \sigma^2 \mathbf{M} \Big) \rho^n + \tau s \Big( \frac{1}{\Delta t} \mathbf{M} + \mathbf{D} + \sigma \mathbf{M} \Big) \\ &\frac{1}{\Delta t} \Big( 2\mathbf{M} + \tau \Big( \frac{\mathbf{M}}{\Delta t} + \mathbf{D} + \sigma \mathbf{M} \Big) \Big) \Delta \rho_2 &= \mathbf{f}^{n+1/2} - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^{n+1/2} \\ &+ \tau \Big( \frac{1}{\Delta t} \mathbf{C} + \mathbf{B} + \sigma \mathbf{C} + \frac{\sigma}{\Delta t} \mathbf{M} + \sigma \mathbf{D} + \sigma^2 \mathbf{M} \Big) \rho^{n+1/2} + \tau s \Big( \frac{1}{\Delta t} \mathbf{M} + \mathbf{D} + \sigma \mathbf{M} \Big) \end{aligned}$$

Finally the linear system to be solved can be written as follows,

$$\mathbf{A}\Delta\rho_1 = \mathbf{F}_1\rho^n$$
$$\mathbf{A}_2\Delta\rho_2 = \mathbf{F}_2\rho^{n+1/2}$$

where the values of  $\rho$  can be computed from  $\rho^{n+1} = \rho^n + \Delta \rho_2$ . The details of the matrices for different methods are described in the following sections.

$$\begin{aligned} \mathbf{A}_1 &= \frac{2}{\Delta t} \mathbf{M} \\ \mathbf{F}_1 &= \mathbf{f}^n - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^n \\ \mathbf{A}_2 &= \frac{1}{\Delta t} \mathbf{M} \\ \mathbf{F}_2 &= \mathbf{f}^{n+1/2} - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \rho^{n+1/2} \end{aligned}$$

SUPG

$$\begin{aligned} \mathbf{A}_1 &= \frac{1}{\Delta t} (2\mathbf{M} + \tau \mathbf{D}) \\ \mathbf{F}_1 &= \mathbf{f}^n - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D}))\rho^n + \tau s \mathbf{D} \\ \mathbf{A}_2 &= \frac{1}{\Delta t} (\mathbf{M} + \tau \mathbf{D}) \\ \mathbf{F}_2 &= \mathbf{f}^{n+1/2} - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau (\mathbf{B} + \sigma \mathbf{D}))\rho^{n+1/2} + \tau s \mathbf{D} \end{aligned}$$

 $\mathbf{GLS}$ 

$$\begin{aligned} \mathbf{A}_{1} &= \frac{1}{\Delta t} \Big( 2\mathbf{M} + \tau \Big( \frac{\mathbf{M}}{\Delta t} + \mathbf{D} + \sigma \mathbf{M} \Big) \Big) \\ \mathbf{F}_{1} &= \mathbf{f}^{n} - \Big( \Big( 1 + \frac{\tau}{\Delta t} + r\sigma \Big) (\mathbf{C} + \sigma \mathbf{M}) + \mathbf{K} + \tau (\mathbf{B} + r\sigma \mathbf{D}) \Big) \rho^{n} + \tau s \Big( \frac{1}{\Delta t} \mathbf{M} + \mathbf{D} + \sigma \mathbf{M} \Big) \\ \mathbf{A}_{2} &= \frac{1}{\Delta t} \Big( \mathbf{M} + \tau \Big( \frac{\mathbf{M}}{\Delta t} + \mathbf{D} + \sigma \mathbf{M} \Big) \Big) \\ \mathbf{F}_{2} &= \mathbf{f}^{n+1/2} - \Big( \Big( 1 + \frac{\tau}{\Delta t} + r\sigma \Big) (\mathbf{C} + \sigma \mathbf{M}) + \mathbf{K} + \tau (\mathbf{B} + r\sigma \mathbf{D}) \Big) \rho^{n+1/2} + \tau s \Big( \frac{1}{\Delta t} \mathbf{M} + \mathbf{D} + \sigma \mathbf{M} \Big) \end{aligned}$$

#### **Implicit Pade**

Considering the implicit pade method, the compact weak form can be written as follows,

$$\left(w, \frac{\Delta\rho}{\Delta t}\right) - \left(w, \mathbf{W}\mathcal{L}(\Delta\rho)\right) + \sum_{e} \int_{\Omega^{e}} \mathcal{P}(w)\tau \mathcal{R}(\Delta\rho)d\Omega = \left(w, \mathbf{w}(s^{n} - \mathcal{L}(\rho^{n}))\right) + \left(w, \mathbf{W}\Delta s\right)$$

The matrix form of different methods is described in the following sections.

#### Galerkin Method

$$\left[\frac{1}{\Delta t}\mathbf{M} + (\mathbf{C} + \mathbf{K} + \sigma\mathbf{M})\mathbf{W}\right]\Delta\rho = (\mathbf{w}\mathbf{f}^n + \mathbf{W}\Delta\mathbf{f}) - (\mathbf{C} + \mathbf{K} + \sigma\mathbf{M})\mathbf{w}\rho^n$$

Derivation

#### Galerkin Method with stabilization

$$\left[\frac{1}{\Delta t}\mathbf{M} + \left(\mathbf{C} + \mathbf{K} + \sigma\mathbf{M}\right)\mathbf{W}\right]\Delta\rho + \sum_{e}\int_{\Omega^{e}}\mathcal{P}(w)\tau\mathcal{R}(\Delta\rho)d\Omega = (\mathbf{w}\mathbf{f}^{n} + \mathbf{W}\Delta\mathbf{f}) - (\mathbf{C} + \mathbf{K} + \sigma\mathbf{M})\mathbf{w}\rho^{n}$$

SUPG stabilization term,

$$\sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho) d\Omega = (\mathbf{W}(a \cdot \nabla)w) \tau \Big[ \frac{\Delta \rho}{\Delta t} - \mathbf{W} \frac{\partial \Delta \rho}{\partial t} - \mathbf{w} \frac{\partial \rho^{n}}{\partial t} \Big]$$

The matrix form of SUPG can be written as follows,

$$\begin{bmatrix} \frac{1}{\Delta t} \mathbf{M} + (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \mathbf{W} + \tau \mathbf{W} (\frac{1}{\Delta t} \mathbf{D} + \mathbf{W} (\mathbf{B} + \sigma \mathbf{D})) \end{bmatrix} \Delta \rho$$
  
=  $(\mathbf{w} \mathbf{f}^n + \mathbf{W} \Delta \mathbf{f}) - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \mathbf{w} \rho^n + \tau \mathbf{W} (\mathbf{w} (\mathbf{B} + \sigma \mathbf{D}) \rho^n - \mathbf{D} (\mathbf{w} s^n + \Delta s))$ 

GLS stabilization term,

$$\sum_{e} \int_{\Omega^{e}} \mathcal{P}(w) \tau \mathcal{R}(\Delta \rho) d\Omega = \left[ \frac{w}{\Delta t} + \mathbf{W}((a \cdot \nabla)w - \nabla \cdot (v\nabla w) + \sigma w) \right] \tau \left[ \frac{\Delta \rho}{\Delta t} - \mathbf{W} \frac{\partial \Delta \rho}{\partial t} - \mathbf{w} \frac{\partial \rho^{n}}{\partial t} \right]$$

The matrix form of GLS can be written as follows,

$$\begin{split} &\left[\frac{1}{\Delta t}\mathbf{M} + \left(\mathbf{C} + \mathbf{K} + \sigma\mathbf{M}\right)\mathbf{W} + \tau \left[\frac{1}{\Delta t}\left(\frac{1}{\Delta t}\mathbf{M} + \mathbf{W}\mathbf{C} + \sigma\mathbf{W}\mathbf{M}\right)\right. \\ &\left. + \mathbf{W}\left(\frac{1}{\Delta t}\mathbf{D} + \mathbf{W}\mathbf{B} + \sigma\mathbf{W}\mathbf{D} + \frac{\sigma}{\Delta t}\mathbf{M} + \sigma\mathbf{W}\mathbf{C} + \sigma^{2}\mathbf{W}\mathbf{M}\right)\right]\right]\Delta\rho \\ &= \left(\mathbf{w}\mathbf{f}^{n} + \mathbf{W}\Delta\mathbf{f}\right) - \left[\mathbf{C} + \mathbf{K} + \sigma\mathbf{M} + \tau \left(\frac{q}{\Delta t}(\mathbf{C} + \sigma\mathbf{M}) + \mathbf{W}(\mathbf{B} + \sigma\mathbf{D} + \sigma\mathbf{C} + \sigma^{2}\mathbf{M})\right)\right]\mathbf{w}\rho^{n} \\ &- \tau \left(\mathbf{w}s^{n} + \mathbf{W}\Delta s\right) \left(\frac{1}{\Delta t}\mathbf{M} + \mathbf{D} + \sigma\mathbf{M}\right) \end{split}$$

Finally linear system to be solved can be written as follows,

$$\mathbf{A} \Delta \rho = \mathbf{F}$$

Similar to the previous case, the values of  $\rho$  can be computed from  $\rho^{n+1} = \rho^n + \Delta \rho$ . The details of the matrices for different methods are described in the following sections.

#### Matrix form of Galerkin method

$$\mathbf{A} = \frac{1}{\Delta t} \mathbf{M} + (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \mathbf{W}$$
$$\mathbf{F} = \mathbf{w}s^n + \mathbf{W}\Delta s - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \mathbf{w}\rho^n$$

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## Matrix form of SUPG

$$\mathbf{A} = \frac{1}{\Delta t} \mathbf{M} + (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M}) \mathbf{W} + \tau \mathbf{W} \left( \frac{1}{\Delta t} \mathbf{D} + \mathbf{W} (\mathbf{B} + \sigma \mathbf{D}) \right)$$
$$\mathbf{F} = (1 + \tau \mathbf{W} \mathbf{D}) (\mathbf{w} s^n + \mathbf{W} \Delta s) - (\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau \mathbf{W} (\mathbf{B} + \sigma \mathbf{D})) \mathbf{w} \rho^n$$

Matrix form of GLS

$$\begin{split} \mathbf{A} &= \frac{1}{\Delta t} \Big( \Big( 1 + \tau \frac{1}{\Delta t} + r \sigma \mathbf{W} \Big) \mathbf{M} + \tau \mathbf{W} \mathbf{C} \Big) \\ &+ \Big( \mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau \Big( \frac{1}{\Delta t} \mathbf{D} + \frac{\sigma}{\Delta t} \mathbf{M} + \mathbf{W} (\mathbf{B} + \sigma \mathbf{D} + \mathbf{C}) + \sigma^2 \mathbf{M} ) \Big) \Big) \mathbf{W} \end{split}$$

$$\begin{aligned} \mathbf{F} &= \Big(1 + \tau \Big(\frac{1}{\Delta t}\mathbf{M} + \mathbf{D} + \sigma \mathbf{M}\Big)\Big)(\mathbf{w}s^n + \mathbf{W}\Delta s) \\ &- \Big(\mathbf{C} + \mathbf{K} + \sigma \mathbf{M} + \tau \Big(\frac{1}{\Delta t}(\mathbf{C} + \sigma \mathbf{M}) + \mathbf{W}(\mathbf{B} + \sigma(\mathbf{D} + \mathbf{C}) + \sigma^2 \mathbf{M})\Big)\Big)\mathbf{w}\rho^n \end{aligned}$$

# 2. Steady State Problem

The domain under consideration is  $\Omega = (0,2) \times (0,3) \in \mathbb{R}^2$ . The boundary  $\Gamma$ , with Dirichlet and Neumann boundary conditions such that  $\Gamma = \Gamma_D \cup \Gamma_N$ , is defined by the following closed set as,

$$\begin{split} \Gamma_1 &= (0,0) \times (0,3/2) \\ \Gamma_2 &= (0,0) \times (3/2,3) \\ \Gamma_3 &= (0,2) \times (3,3) \\ \Gamma_4 &= (2,2) \times (0,3) \\ \Gamma_5 &= (0,2) \times (0,0) \end{split}$$

The domain and its boundaries is presented in Figure 2.1.



Figure 2.1: Domain with boundaries

Considering the steady-state case and solving the problem with linear and quadratic elements and the following convective velocity, diffusion parameter, reaction and source:

(1)  $a = (-1, 0), \nu = 10^{-3}, \sigma = 10^{-3}, s = 0$ , number of elements is 20 per direction.

For this case the Peclet number is 62.5 when the number of elements is 20 per direction.



Figure 2.2: Results with linear elements

As it can be seen from Figures 2.2a and 2.3a that the Galerkin solution is corrupted by non-physical oscillations when the Péclet number is larger than one. It can be observed that when the stabilization term is included to the Galerkin weak form, the results are smooth and stable without any oscillations.



Figure 2.3: Results with quadratic elements

(2)  $a = (-10^{-3}, 0), \nu = 10^{-3}, \sigma = 1, s = 0$ 

For this case the Peclet number is 0.0625 when a mesh with 20 elements per direction is considered.



Figure 2.4: Results with linear elements

This test is a reaction dominant problem. As the Péclet number is automatically satisfied due to the parameter settings. Galerkin and Galerkin with SUPG or GLS all give stable results regardless the size or the mesh, as presented in Figures 2.4 and 2.5.



Figure 2.5: Results with quadratic elements

(3)  $a = (-1, 0), \nu = 10^{-3}, \sigma = 0, s = 1$ 

For this case the Peclet number is 0.0625 when a mesh with 20 elements per direction is considered.



Figure 2.6: Results with linear elements

This test is a source term dominate problem. As the Péclet number is also automatically satisfied due to the parameter settings. Galerkin and Galerkin with SUPG or GLS all give stable results regardless the size or the mesh, as presented in Figures 2.6 and 2.7. As there is a constant source term inside the domain, the solution at the nodes tends to go up and have very large displacements (as in the Figures 2.6 and 2.7, the magnitude of the displacement is at around 600 to 800). As the boundary  $\Gamma_2$  and  $\Gamma_4$  is bounded, assigned the Dirichlet boundary condition, those boundaries are fixed which can also be observed in the figures.



Figure 2.7: Results with quadratic elements